$\Rightarrow$ ambiguity of ensemble interpretation!

In fact, there are infinitely many ensembles for the same density operator!

Even the number of terms can vary:

E.g.: $|\psi\rangle = \frac{\alpha|00\rangle + \beta|11\rangle}{\sqrt{2}} + \frac{\alpha|02\rangle + \beta|13\rangle}{\sqrt{3}}$

Measure in basis $|0\rangle, |1\rangle, \frac{|2\rangle \pm |3\rangle}{\sqrt{2}} =: |\pm\rangle$

$\rightarrow$ combination of the two previous schemes!

$$\Rightarrow \quad \rho_A = \underset{\overset{\shortparallel}{|\alpha|^2/2}}{p_0}|0\rangle\langle 0| + \underset{\overset{\shortparallel}{|\beta|^2/2}}{p_1}|1\rangle\langle 1| + \underset{\overset{\shortparallel}{1/4}}{p_+}|\psi_+\rangle\langle\psi_+| + \underset{\overset{\shortparallel}{1/4}}{p_-}|\psi_-\rangle\langle\psi_-|$$

How are different ensembles related?

Theorem: Let $\rho = \sum p_i |\psi_i\rangle\langle\psi_i| = \sum q_j |\phi_j\rangle\langle\phi_j|$.

Then, there is a unitary $U = (u_{ij})$ s.th.

$$\sqrt{p_i}|\psi_i\rangle = \sum u_{ij}\sqrt{q_j}\,|\phi_j\rangle,$$

and vice versa. (If the number of i's and j's is different, pad the smaller one with zero vectors!)

Proof:

"$\Leftarrow$": Let $\sqrt{p_i}\,|\psi_i\rangle = \sum u_{ij}\sqrt{q_j}\,|\phi_j\rangle$.

Then $\sum_i p_i|\psi_i\rangle\langle\psi_i| = \sum_i \Big(\sum_j u_{ij}\sqrt{q_j}\,|\phi_j\rangle\Big)\Big(\sum_{j'} u_{ij'}^*\sqrt{q_{j'}}\langle\phi_{j'}|\Big)$

$$= \sum_{jj'} \sqrt{q_j}\,|\phi_j\rangle\langle\phi_{j'}|\sqrt{q_{j'}}\;\underbrace{\Big(\sum_i u_{ij'}^* u_{ij}\Big)}_{=\delta_{jj'}}$$

$$= \sum_j q_j\,|\phi_j\rangle\langle\phi_j|$$

"$\Rightarrow$": First, assume $|\phi_j\rangle$ is an eigenbasis. Define

$$u_{ij} = \langle\phi_j|\psi_i\rangle\cdot\frac{\sqrt{p_i}}{\sqrt{q_j}}$$

Then, $\sum_j u_{ij}\sqrt{q_j}\,|\phi_j\rangle = \sum_j \sqrt{q_j}\,|\phi_j\rangle\langle\phi_j|\psi_i\rangle\,\frac{\sqrt{p_i}}{\sqrt{q_j}} = \sqrt{p_i}\,|\psi_i\rangle$

and $\sum_i u_{ij}u_{ij'}^* = \sum_i \langle\phi_j|\psi_i\rangle\langle\psi_i|\phi_{j'}\rangle\,\frac{p_i}{\sqrt{q_j q_{j'}}}$

$$= \underbrace{\langle\phi_j|\rho|\phi_{j'}\rangle}_{=q_j\delta_{jj'}}\,\frac{1}{\sqrt{q_j q_{j'}}} = \delta_{jj'}$$

$\Rightarrow$ u_{ij} has orthogonal columns $\Rightarrow$ can be extended to unitary (by padding $|\phi_i\rangle$ with zero vectors).

General case: Go via eigenbasis & combine unitaries! ∎

3. Schmidt decomposition and purifications

Consider bipartite state $|\psi\rangle_{AB}$, and let

$$\mathrm{tr}_B |\psi\rangle\langle\psi| = \rho_A = \sum p_i |i\rangle_A \langle i|_A \Rightarrow |i\rangle_A \text{ ONB.}$$

Choose an ONB $|a_j\rangle_B$ for B, and expand

$$|\psi\rangle_{AB} = \sum c_{ij} |i\rangle_A |a_j\rangle_B$$

$$= \sum |i\rangle_A |b_i\rangle_B \,, \quad |b_i\rangle = \sum c_{ij} |a_j\rangle$$

↑ no ONB!

Now $\sum p_i |i\rangle\langle i| = \mathrm{tr}_B |\psi\rangle\langle\psi| = \mathrm{tr}_B \left(\sum_{ii'} |i\rangle\langle i'|_A \, |b_i\rangle\langle b_{i'}|_B \right)$

$$= \sum_{j, ii'} |i\rangle\langle i'| \underbrace{\langle a_j | b_i\rangle \langle b_{i'} | a_j\rangle}_{\sum_j :\; = \langle b_{i'} | b_i\rangle}$$

$$= \sum \langle b_{i'} | b_i \rangle \, |i\rangle\langle i'|$$

$|i\rangle\langle i'|$ is a basis for the space of matrices (= linear maps):

$$\Rightarrow \langle b_{i'} | b_i \rangle = \delta_{i'i} \, p_i$$

$\Rightarrow |i\rangle_B := \frac{1}{\sqrt{p_i}} |b_i\rangle$ is ONB for B

different from $|i\rangle_A$!

$$\Rightarrow \boxed{\begin{array}{c} |\psi\rangle_{AB} = \sum_i \sqrt{p_i}\, |i\rangle_A |i\rangle_B \\[2ex] \text{with } |i\rangle_A,\ |i\rangle_B \text{ ONBs} \end{array}}$$

"Schmidt decomposition" with Schmidt coefficients $\sqrt{p_i}$.

Note: $\rho_B = \mathrm{tr}_A |\psi\rangle\langle\psi| = \sum_i p_i |i\rangle_B\langle i|_B$

$\Rightarrow |i\rangle_B$ is the eigenbasis of ρ_B !

p_i non-degenerate $\Rightarrow$ Schmidt decomposition obtained by pairing up eigenvectors of ρ_A and ρ_B !

Important consequence: Eigenvalues of ρ_A and ρ_B are equal !

How is the Schmidt decomp. related to other expansions?

$$|\psi\rangle = \sum c_{ij} \, |x_i\rangle_A \, |y_j\rangle_B$$

ONB

$$= \sum \sqrt{p_k} \, |k\rangle_A \, |k\rangle_B$$

$\Longrightarrow$ $\exists$ unitaries u_{ik}, v_{jk} s.th.

$$|k\rangle_A = \sum u_{ik} \, |x_i\rangle_A ; \quad |k\rangle_B = \sum v_{jk}^* \, |y_j\rangle_B$$

(pad p_k w/ zeros if necessary).

$\xRightarrow[\text{+ lin. indep.}]{\text{input above}}$
$$c_{ij} = \sum_k u_{ik} \sqrt{p_k} \, v_{jk}^* ,$$

or

$$\underbrace{(u_{ik})}_{C = U} \underbrace{\begin{pmatrix} \sqrt{p_1} & & \\ & \ddots & \\ & & \end{pmatrix}}_{\cdot D} \underbrace{(v_{jk})}_{\cdot V^\dagger}$$

$$C = U \cdot D \cdot V^\dagger$$; U, V unitary, D diagonal

$\boxed{\text{"singular value decomposition" (SVD)}}$

Remark: Any two states $|\phi\rangle, |\psi\rangle$ w/ identical Schmidt coefficients are related by local unitaries, i.e.:

$$\exists U,V \text{ s.th. } |\phi\rangle = (U \otimes V)|\psi\rangle.$$

I.e.: All non-local properties are encoded in the p_i!

Proof:

$$|\phi\rangle = \sum \sqrt{p_i}\, |\phi_i^A\rangle \otimes |\phi_i^B\rangle$$

$$|\psi\rangle = \sum \sqrt{p_i}\, |\psi_i^A\rangle \otimes |\psi_i^B\rangle$$

$|\phi_i^A\rangle, |\psi_i^A\rangle$ orthonormal $\Rightarrow \exists U : |\phi_i^A\rangle = U|\psi_i^A\rangle \ \forall i$

$|\phi_i^B\rangle, |\psi_i^B\rangle$ —"— $\Rightarrow \exists V : |\phi_i^B\rangle = V|\psi_i^B\rangle \ \forall i$

$\boxed{R}$

(Note: If necessary, we have to pad the p_i with zeros and embed Hilbert space in larger one.)

Purifications:

Have seen: Bipartite state $|\psi\rangle_{AB}$ w/ access to A only

$\Rightarrow$ described by ρ_A, $\rho_A \geq 0$, $\mathrm{tr}\,\rho_A = 1$

Will now show: Any such ρ_A can be seen as arising from $|\psi\rangle_{AB}$ ("purification")

Let $\rho = \sum p_i |\phi_i\rangle\langle\phi_i|$

need not be orthogonal

Choose $|\psi\rangle_{AB} = \sum \sqrt{p_i}\, |\phi_i\rangle_A |i\rangle_B$

orthonormal.

Then $tr_B |\psi\rangle\langle\psi| = \sum_{k,i,j} \underbrace{\langle k|_B \Big(\sqrt{p_i p_j}\, |\phi_i\rangle_A |i\rangle_B}_{=\delta_{ki}} \langle\phi_j|_A \underbrace{\langle j|_B\Big)|k\rangle_B}_{=\delta_{kj}}$

$= \sum_k p_k |\phi_k\rangle\langle\phi_k|$ ✓

$|\psi\rangle$ is called *purification* of ρ.

Notes:
- Measuring in basis $|i\rangle_B$ prepares ensemble $\{p_i, |\phi_i\rangle\}$
- We can always choose $\dim(\mathcal{H}_B) \leq \dim(\mathcal{H}_A)$ by using eigenvalue decomposition of ρ.
  (In fact, even $\dim \mathcal{H}_B = \#$ non-zero Schmidt coeff.)

Many different purifications exist! How are they related?

Let $|\phi\rangle_{AB}$, $|\psi\rangle_{AB}$ be purifications of ρ_A.

Write both in their Schmidt decomposition:

$$|\phi\rangle = \sum_i \lambda_i \, |\phi_i^A\rangle |\phi_i^B\rangle$$

$$|\psi\rangle = \sum_i \lambda_i \, |\psi_i^A\rangle |\psi_i^B\rangle.$$

We have $\sum \lambda_i |\phi_i^A\rangle\langle\phi_i^A| = \sum \lambda_i |\psi_i^A\rangle\langle\psi_i^A|$

$\Longrightarrow$ $|\phi_i^A\rangle = |\psi_i^B\rangle$ if λ_i non-degenerate

<u>and we know</u> from construction of Schmidt decomp. that we can choose $|\phi_i^A\rangle = |\psi_i^A\rangle \;\forall i$!

Now choose U s.th. $U|\phi_i^B\rangle = |\psi_i^B\rangle \;\forall i$.

$$\Longrightarrow \quad |\psi\rangle = (\mathbb{1} \otimes U)\,|\phi\rangle.$$

All purifications are related by a unitary on the purifying system.

(<u>Note</u>: This can be seen as a reformulation of the unitary relation of ensemble decompositions.)

1. Unitary evolution of mixed states

How does a mixed state ρ_A evolve under a unitary U_A?

Consider purification $|\psi\rangle_{AB}$; $\mathrm{tr}_B |\psi\rangle\langle\psi| = \rho_A$.

$$|\psi\rangle \longmapsto (U_A \otimes \mathbb{1}_B)|\psi_{AB}\rangle$$

$$\Rightarrow \rho_A = \mathrm{tr}_B |\psi\rangle\langle\psi| \longmapsto \mathrm{tr}_B \left[(U_A \otimes \mathbb{1}_B)|\psi_{AB}\rangle\langle\psi_{AB}|(U_A^\dagger \otimes \mathbb{1}_B)\right]$$

$$= U_A \cdot \mathrm{tr}_B \left[(\mathbb{1}_A \otimes \mathbb{1}_B)|\psi_{AB}\rangle\langle\psi_{AB}|(\mathbb{1}_A \otimes \mathbb{1}_B)\right] U_A^\dagger$$

$$= \underline{\underline{U_A \rho_A U_A^\dagger}}.$$

2. Measurement of mixed states

Projective measurement E_u:

Have seen: $p_u = \mathrm{tr}[E_u \rho_A]$.

Post-measurement state:

$$\rho_{A,u} = \frac{1}{p_u} \mathrm{tr}_B \left((E_u \otimes \mathbb{1})|\psi\rangle\langle\psi|(E_u^\dagger \otimes \mathbb{1})\right)$$

$$= \underline{\underline{\frac{1}{p_u} E_u \rho_A E_u^\dagger}}$$

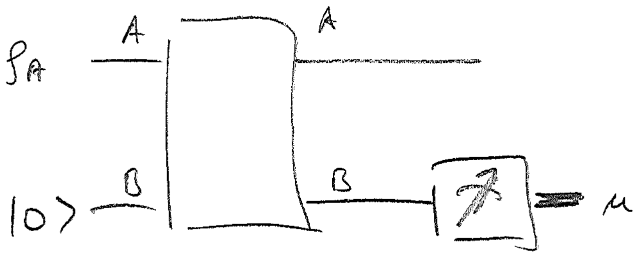
4. POVM measurements

Have seen: additional system B → more rich situation

What measurements can we do by adding an extra system?

Idea:

Add "ancilla" B (in state $|0\rangle_B$), act w/ unitary on AB, and measure B in computational basis $|0\rangle, \dots, |d-1\rangle$.



Post-measurement state (unnormalized):

$$\tilde{\rho}_u^A = \langle u|_B \, U \left(\rho_A \otimes |0\rangle_B \langle 0|_B \right) U^\dagger |u\rangle_B$$

$$= M_u \rho_A M_u^\dagger \,, \quad \text{with } M_u := \langle u|_B \, U |0\rangle_B .$$

$$\equiv \left(\mathbb{1}_A \otimes \langle u|_B \right) U \left(\mathbb{1}_A \otimes |u\rangle_B \right)$$

and $p_u = tr\left(\tilde{\rho}_u^A\right) = tr\left(M_u \rho_A M_u^\dagger\right) = tr\left(M_u^\dagger M_u \rho_A\right)$

$\rho_u^A = \frac{1}{p_u} \tilde{\rho}_u^A$ post-meas. state.

What properties does Π_u have?

$$\underline{\underline{\sum \Pi_u^\dagger \Pi_u}} = \sum_u \langle 0|_B \, \underbrace{U^\dagger \underbrace{|u\rangle_B \langle u|_B}_{=\mathbb{1}} U}_{=\mathbb{1}} |0\rangle_B = \langle 0|_B \mathbb{1}_{AB} |0\rangle_B$$

$$\underline{\underline{= \mathbb{1}_A}} .$$

(Also follows from $1 = \sum p_u = \sum \mathrm{tr}(\Pi_u^\dagger \Pi_u \rho_A) = \mathrm{tr}(\sum \Pi_u^\dagger \Pi_u \rho_A)$ $\forall \rho_A$)

A set of $\{\Pi_u\}$ (or $\{\Pi_u^\dagger \Pi_u\}$ w/ $\sum \Pi_u^\dagger \Pi_u = \mathbb{1}$ is called a "positive operator-valued measure" (POVM), and the corresp. measurement a <u>POVM measurement</u>.

Can any set Π_u w/ $\sum \Pi_u^\dagger \Pi_u = \mathbb{1}$ be realized by extensions + unitaries?

$$\begin{pmatrix} \Pi_0 \\ \vdots \\ \\ \\ \Pi_{d-1} \end{pmatrix} \quad \sum \Pi_u^\dagger \Pi_u = \mathbb{1} \quad \Longrightarrow \quad \text{matrix w/ orthogonal columns} \quad \Longrightarrow \quad \ldots$$

$\Rightarrow$ can be extended to unitary $\mathcal{U}$

$$\mathcal{U} = \begin{array}{c} \\ \langle 0|_B \\ \langle 1|_B \\ \vdots \\ \langle d|_B \end{array} \begin{array}{c} |0\rangle_B \\ \left(\begin{array}{c|cccc} M_0 & \cdot & \cdot & \cdot & \cdot \\ \hline M_1 & \cdot & \cdot & \cdot & \cdot \\ \hline \vdots & & & & \\ \hline M_{d-1} & \cdot & \cdot & \cdot & \cdot \end{array} \right) \end{array}$$

i.e.: $\langle n|_B\, \mathcal{U}\, |0\rangle_B = M_n .$

$\Rightarrow$ measurement $\{M_n\}$ can be realized by unitary $\mathcal{U}$ & projective measurement!

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5. General evolution – superoperators

What evolutions can we realize by evolving a larger system with a unitary?